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Level Shifts and Inelastic Electron Scattering in Dense Plasmas

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20. ABSTRACT (Continued)

transition probabilities, and electron collision cross sections of Ne^{+9} for temperature and 200 and 500 eV for an electron density range of $1 - 6 \times 10^{24} \text{ cm}^{-3}$, and of Ar^{+17} for temperatures of 1000 and 2000 eV and electron densities from 2×10^{26} to $8 \times 10^{26} \text{ cm}^{-3}$. In the low-density region, level shifts are obtained for H and He^3 .

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10 to the 25th Power

Ne (9+)

Ar (17+)

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LEVEL SHIFTS AND INELASTIC ELECTRON SCATTERING IN DENSE PLASMAS

I. INTRODUCTION

The plasma polarization shift of spectral lines remains a basic and controversial effect. Griem¹ tried to explain the blue shifts for the resonance lines of ionized helium by considering the perturbation of the upper levels by free plasma electrons. An alternate approach involves the solution of the Schrodinger equation for the bound electrons in the Debye-Huckel potential. This leads to red shifts of the lines because it causes large shifts of the lower levels. Experimentally, evidence has been reported for blue shifts² of Lyman lines and red shifts³ for Balmer lines for He II, but shifts measured for other similar ionized emitters are much smaller or zero.

Theimer and Kepple⁴ have shown that the theory using the Debye-Huckel potential is inadequate because it ignores the reaction of plasma electrons to the presence of the bound electron. Their self-consistent calculation for a hydrogen plasma indicates much smaller level shifts than those predicted by previous theories. More recently, an analogous treatment was adopted by Rozsnyai⁵ and Skupsky⁶ with similar results. In these theories the free electron gas was treated classically and the energy levels were obtained from the solution of the Schrodinger equation.

In the present investigation we obtained level shifts, transition probability coefficients and collision cross sections for Ne⁺⁹ and Ar⁺¹⁷ in a plasma with electron density ranging from 10^{24} to $6 \times 10^{24} \text{ cm}^{-3}$ (for Ne⁺⁹) and from 2×10^{25} to $8 \times 10^{25} \text{ cm}^{-3}$ (for Ar⁺¹⁷) using a quantum-mechanical description of the plasma electrons. The theory in a simplified form was applied to the low-density region and level shifts were obtained for H and He⁺.

II. DESCRIPTION OF THE METHOD

We consider an isolated impurity ion with nuclear charge Z immersed in a fully ionized hydrogen plasma. For simplicity all electric charges are assumed to have a spherically symmetric charge distribution. In addition, the positive charge due to protons is continuously distributed. This last assumption is probably the most drastic simplification that we have adopted.

Two types of ions will be studied: completely stripped ions and one-electron hydrogenic ions. In the latter case, it is assumed that in a dense hot plasma the average local charge density due to the bound electron can be written as (atomic units are used throughout the paper, unless indicated)

$$\rho_b = - (4\pi r^2)^{-1} \sum_{n\ell} b_{n\ell} P_{n\ell}^2(r), \quad (1)$$

where $b_{n\ell}$ are the occupation numbers, $P_{n\ell}(r)$ are normalized radial wave functions, and $\sum_{n\ell} b_{n\ell} = 1$. In order for this assumption to be valid it is necessary that the average time between collisions leading to ionization and recombination be substantially larger than the time between collisions that change the state of excitation. Generally, the occupation numbers represent an average state of excitation of the ion and are determined by all possible collisional and radiative processes involving the bound electron. Due to the complexity of this situation, simplifying assumptions about $b_{n\ell}$ will be adopted.

If ρ_e and ρ_p represent local charge densities due to the free electrons and protons, the electrostatic potential $V(r)$ at the distance r from the nucleus with charge Z is then given by

$$V(r) = Z r^{-1} + 4\pi \left[r^{-1} \int_0^r r'^2 (\rho_e + \rho_p + \rho_b) dr' + \int_r^\infty r' (\rho_e + \rho_p + \rho_b) dr' \right]. \quad (2)$$

At large distances from the ion, $\rho_b = 0$ and the plasma is neutral, so that

$$-\rho_e = \rho_p \equiv \rho_\infty \equiv N_e. \quad (3)$$

The positive charge distribution is described by classical Boltzmann statistics, viz.

$$\rho_p = \rho_\infty \exp(-V/k_B T), \quad (4)$$

where $V(r)$ is given by (2), T is the temperature and k_B the Boltzmann constant.

The free electrons are represented by a Fermi-Dirac energy distribution outside a spherical boundary corresponding to the distance r_0 from the nucleus; however, inside this boundary they can be treated quantum-mechanically and described by wave functions which are solutions of the time independent Schrodinger equation. In practical calculations the distance r_0 is taken to be large enough so that plasma at the boundary may be considered neutral and condition (3) valid within numerical accuracy. The wave functions for the free electrons with energy $\frac{1}{2}k^2$ at $r > r_0$ can be expanded in partial waves and the expression for the spherically averaged charge density due to the free electrons at any r is then given by

$$\rho_e = - \int_0^\infty W(k) (kr^2)^{-1} \sum_{\ell=0}^{\infty} (2\ell+1) F_{k\ell}^2(r) dk, \quad (5)$$

where

$$W(k) = \pi^{-2} k^2 \left[1 + \exp \left\{ \left(\frac{1}{2} k^2 - \mu \right) / k_B T \right\} \right]^{-1}. \quad (6)$$

μ is the chemical potential of the free electron gas determined by the condition

$$\int_0^\infty W(k) dk = \rho_\infty \quad (7)$$

and the functions $F_{k\ell}$ are solutions of the equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + 2V(r) - 2V_{ex}(r) - 2V_{corr}(r) + 2V_{ex}(\infty) + 2V_{corr}(\infty) + k^2 \right] F_{k\ell}(r) = 0 \quad (8)$$

with the asymptotic form

$$F_{k\ell}(r) \sim k^{-\frac{1}{2}} \sin(kr + \delta_{k\ell}). \quad (9)$$

The electrostatic potential V is given by (2) and the exchange energy V_{ex} and the correlation energy V_{corr} of a free electron in a plasma were taken from Dharma-wardana^{7,8} and Taylor⁸ and are given in terms of temperature T and local electron density $N_e \equiv \rho_e$:

$$V_{\text{ex}} = -0.4073 r_s^{-1} \tanh(\tau^{-1}), \quad (10)$$

$$V_{\text{corr}} = -0.6109 r_s^{-\frac{1}{2}} (-0.0081 + 1.127 \tau^2 + 2.756 \tau^4) \times (1.0 + 1.291 \tau^2 + 3.593 \tau^4)^{-1} \tanh(\tau^{-\frac{1}{2}}), \quad (11)$$

$$\tau = 2 \left(\frac{4}{9\pi} \right)^{\frac{2}{3}} r_s^2 k_B T,$$

$$r_s^{-1} = \left(\frac{4}{3} \pi n_e \right)^{\frac{1}{3}}.$$

In practice, the integral in (5) is replaced by a summation and an 8-point Gaussian quadrature was used to evaluate ρ_e for each value of r . At large distances, the convergence of the sum over partial waves in (5) is rather slow and we found it necessary to include up to 50 or 70 partial waves, depending on the value of k , to achieve sufficient accuracy for $r < r_0$.

The effect of Fermi degeneracy is taken into account by the distribution function $W(k)$ in (5) for densities equal to ρ_∞ . For the cases studied in this paper the Fermi degeneracy causes only minor deviations from the Maxwell-Boltzmann distribution. Inside the boundary r_0 , where the plasma electrons in our model are described by wave functions and where the local electron densities may reach values substantially larger than ρ_∞ , the effect of degeneracy should be properly taken into account by using an antisymmetric function for the whole system. Due to complications arising from this procedure, we have ignored the possible additional effects of Fermi degeneracy inside r_0 . Also all effects due to relativistic corrections have been ignored since they are probably negligible for light nuclei.

Radial functions P_{nl} of the bound electron satisfy the equation

$$\left[\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + 2V_b(r) + 2E_{nl} \right] P_{nl}(r) = 0. \quad (12)$$

The potential V_b acting on the bound electron is given by (2) with $\rho_b = 0$. The energy shift of a hydrogenic level $n\ell$ due to the plasma polarization is

$$\Delta E_{n\ell} = E_{n\ell} + Z^2(2n^2)^{-1} \quad (13)$$

Equations (1), (2), (4), (5), (8) and (12) should be solved self-consistently with the boundary condition

$$rV(r) \rightarrow 0, P_{n\ell}(r) \rightarrow 0 \quad (14)$$

for $r \rightarrow \infty$. In practice this condition should be satisfied at $r = r_0$.

The equations were solved iteratively starting with hydrogenic $P_{n\ell}$ (for hydrogenic ions) and with $V(r)$ initially replaced by a Debye-Huckel potential. First we found a self-consistent potential (2) while keeping $P_{n\ell}$ unchanged. This procedure requires up to four iterations. Then we used the new form of $P_{n\ell}$ obtained from (12) for the following sequence of iterations. It was found that in all cases presently studied the second sequence of iterations did not lead to any substantial improvement of results and that the first sequence already yielded self-consistent values of $P_{n\ell}$ and $E_{n\ell}$.

III. RESULTS FOR Ne^{+10} , Ne^{+9} and Ar^{+17}

Figure 1 shows two typical examples of the quantity rV for Ne^{+10} , where V is the self-consistent potential (2) with $\rho_b = 0$. These results are compared with the Debye-Huckel theory of plasma screening, which agrees well with the self-consistent potential at distances larger than $2D$, where D is the Debye screening length, but the Debye-Huckel potential is systematically lower in the inner region. The difference appears to increase with decreasing values of D .

The calculations for hydrogen-like Ne^{+9} and Ar^{+17} were performed with the simplifying assumption that the levels $1s$, $2s$ and $2p$ are populated according to Boltzmann statistics and that all occupation numbers $b_{n\ell}$ with $n > 2$ are zero. The local densities $n_e(r)$ and $n_p(r)$ of free electrons and protons for $N_e = 3 \times 10^{24} \text{ cm}^{-3}$ and $T = 200 \text{ eV}$ are displayed on Figs. 2 and 3 for Ne^{+9} . The oscillatory behavior of n_e is caused by interference effects and is mainly due to the slowly moving electrons.

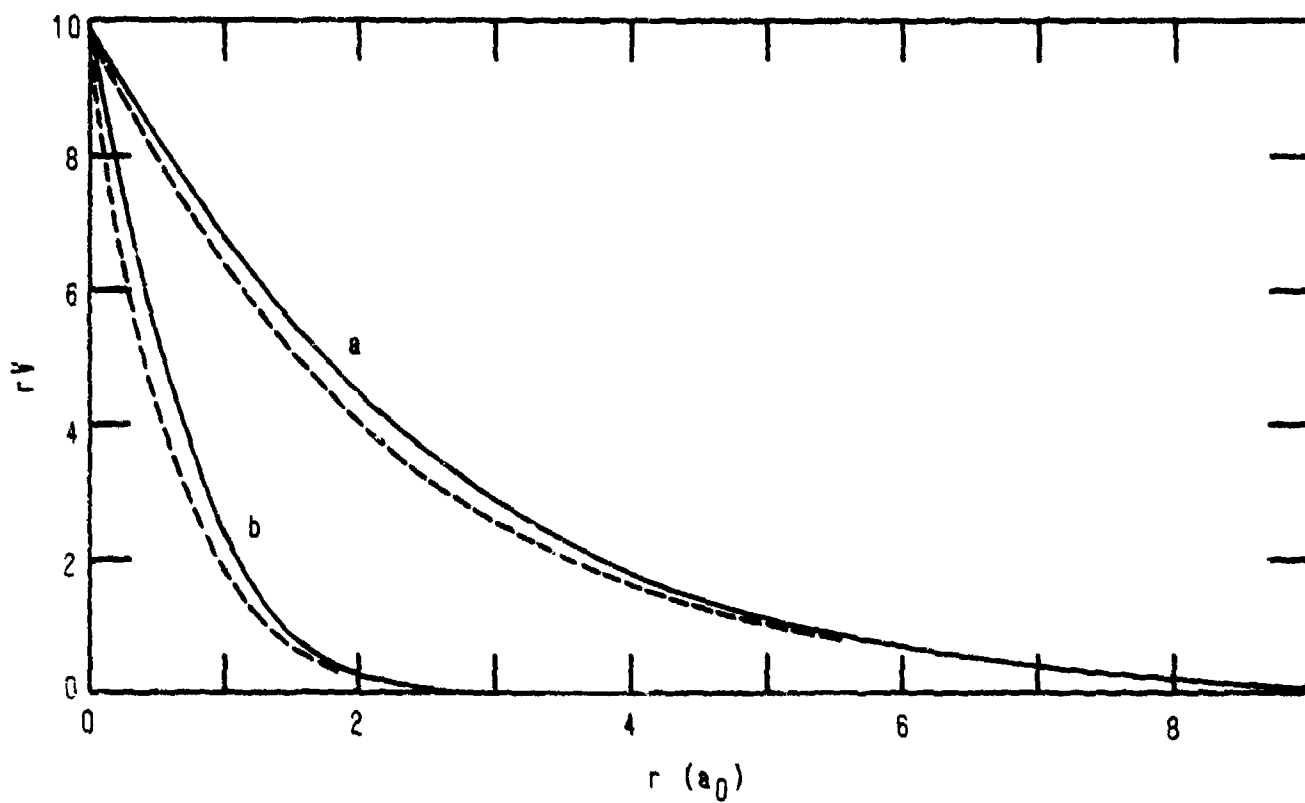


Figure 1. The quantity rV for Ne^{+10} . Full curve - present results;
dashed curve - Debye-Huckel theory.
a - $N_e = 10^{24}$, $T = 500$ eV; b - $N_e = 6 \times 10^{24}$, $T = 200$ eV.

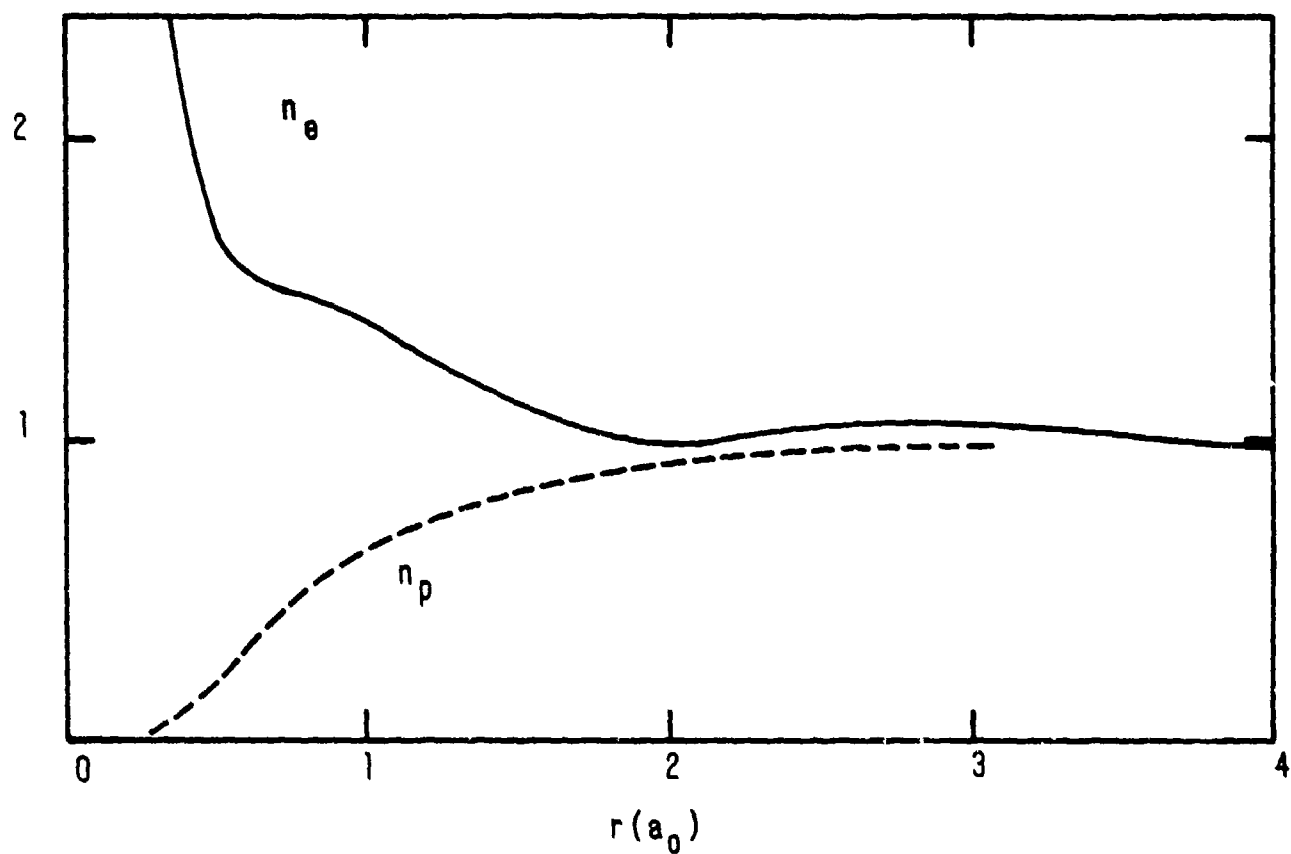


Figure 2. Density distribution of free electrons and protons for Ne^{+9} .
 Densities are normalized to unity at infinity.
 $N_e = 3 \times 10^{24}$, $T = 200$ eV.

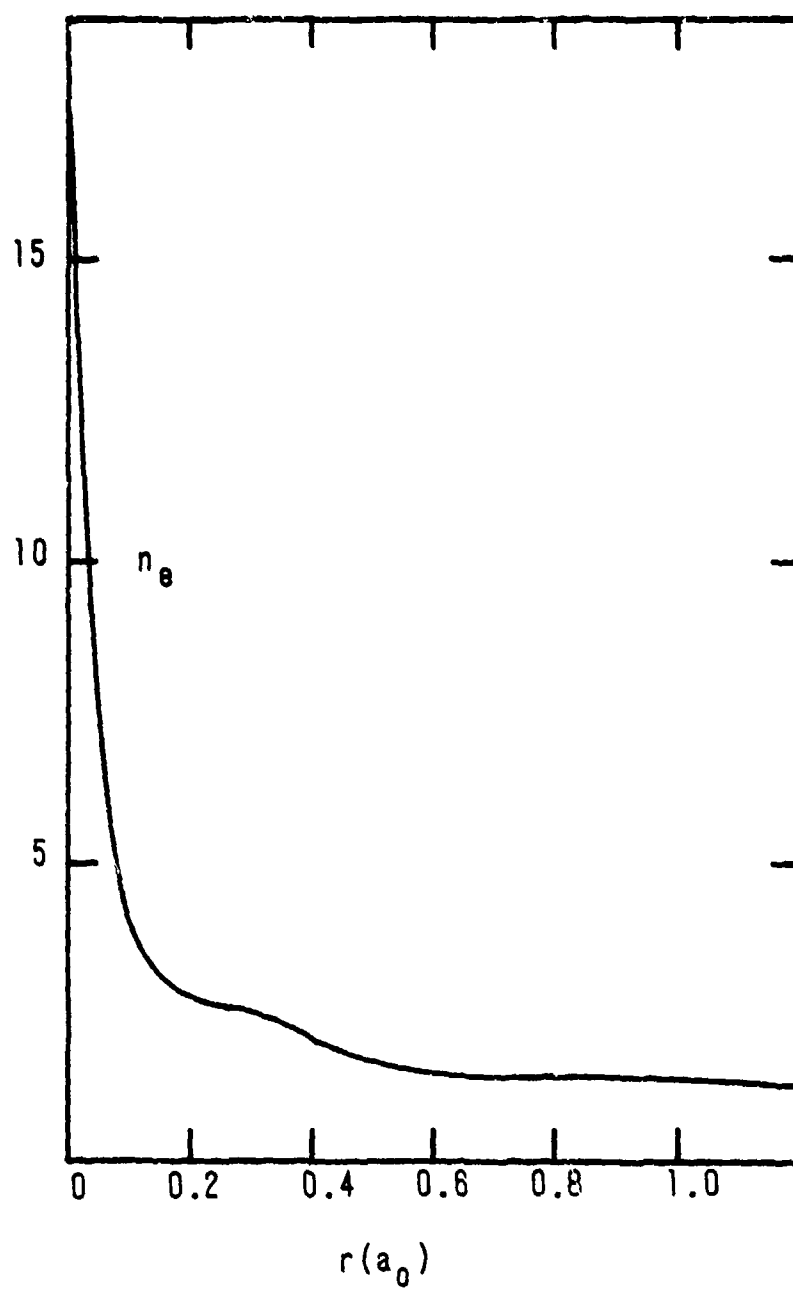


Figure 3. Same as in Figure 2.

Table 1 presents the atomic level shifts (13) for two temperatures and three electron densities N_e . Resulting line shifts of the Lyman α radiation are shown in Figs. 4 and 5. The line shifts are assumed to be equal to the difference of level shifts. The present values of line shifts are slightly larger than the results of Skupsky⁶ who treated the free electrons classically with quantum mechanical corrections to the potential.

Table 2 shows how the Einstein coefficients of transition probability A for the Lyman α line are affected by plasma conditions. A_{Coul} is the coefficient corresponding to the pure Coulomb field, i.e. to $N_e = 0$. The change of transition probabilities is a consequence of the line shift combined with the change of radial functions P_{nl} . In order to ascertain the sensitivity of line shifts to the choice of b_{nl} , we carried out additional calculations for Ne^{+9} with the assumption that only the 1s ground level is occupied. The resulting line shifts were found to be only about 1% smaller than those shown in Fig. 4.

In the present calculations we have ignored all effects related to the time dependent perturbations by plasma electrons and protons. In particular, a possible redistribution of electron velocities inside the boundary r_0 due to electron-electron and electron-proton collisions was not taken into account and effects leading to broadening of spectral lines were also omitted. Thus the results indicate the magnitude of effects caused by plasma polarization alone. In situations where there are only few electrons inside the Debye sphere and collisions do not happen very often, the present treatment should be preferable to the procedures based on statistical considerations for plasma electrons.

The calculation of collision excitation cross sections and rates in a dense plasma should proceed, in principle, along the lines of many-body quantum theory. However, the two-body approximation may still be useful not only for approximate evaluation of excitation rates, but especially because its simplicity allows us to separate various plasma effects.

The change in the value of excitation cross sections and rates in dense plasmas is the result of several causes: (a) changed excitation energy, (b) changed wave functions of atomic electrons, (c) distortion of the incident and scattered waves by the charge cloud around the target ion, (d) modification of the Coulomb interaction potential $|\vec{r}_1 - \vec{r}_2|^{-1} \equiv r_{12}^{-1}$ for the colliding and bound electron by plasma effects, and (3) other effects of many-body interactions.

Table 1
LEVEL SHIFT (eV)

	T(eV)	N_e (cm ⁻³)	1s	2s	2p
Ne X	200	10 ²⁴	122.8	115.6	117.5
		3x10 ²⁴	194.0	173.3	178.5
		6x10 ²⁴	225.5	189.8	198.1
	500	10 ²⁴	90.0	85.5	86.7
		3x10 ²⁴	147.3	134.2	137.5
		6x10 ²⁴	199.6	174.3	180.3
Ar XVIII	1000	2x10 ²⁵	475.8	439.9	449.1
		5x10 ²⁵	702.0	616.4	637.5
		8x10 ²⁵	865.0	736.0	766.4
	2000	2x10 ²⁵	375.8	351.0	357.3
		5x10 ²⁵	563.8	504.5	518.8
		8x10 ²⁵	695.0	602.6	624.3

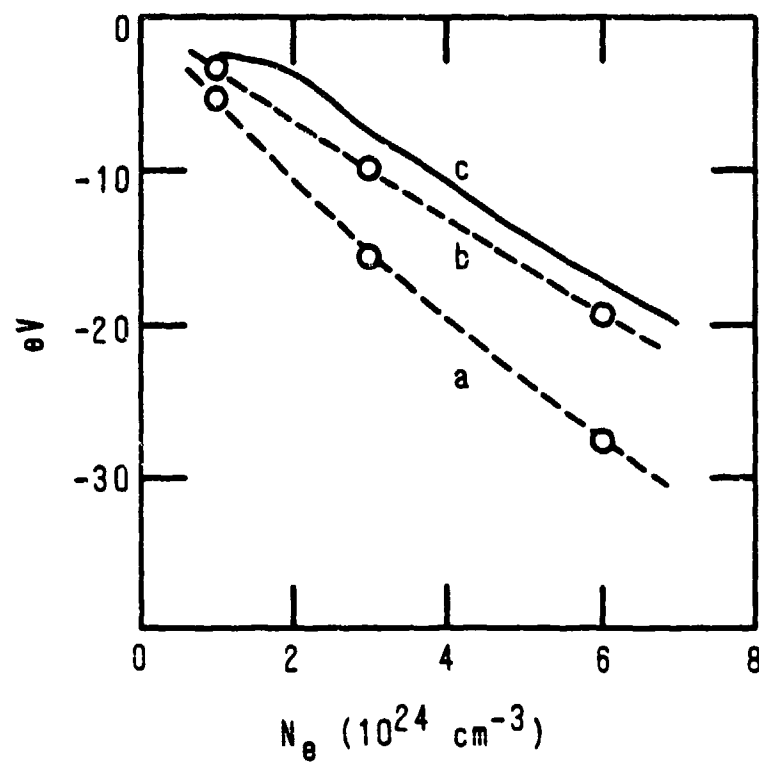


Figure 4. Density dependence of the Ne X Lyman - α line shift.
a - $T = 200$ eV; b - $T = 500$ eV; c - results of Skupsky⁶
($T = 500$ eV).

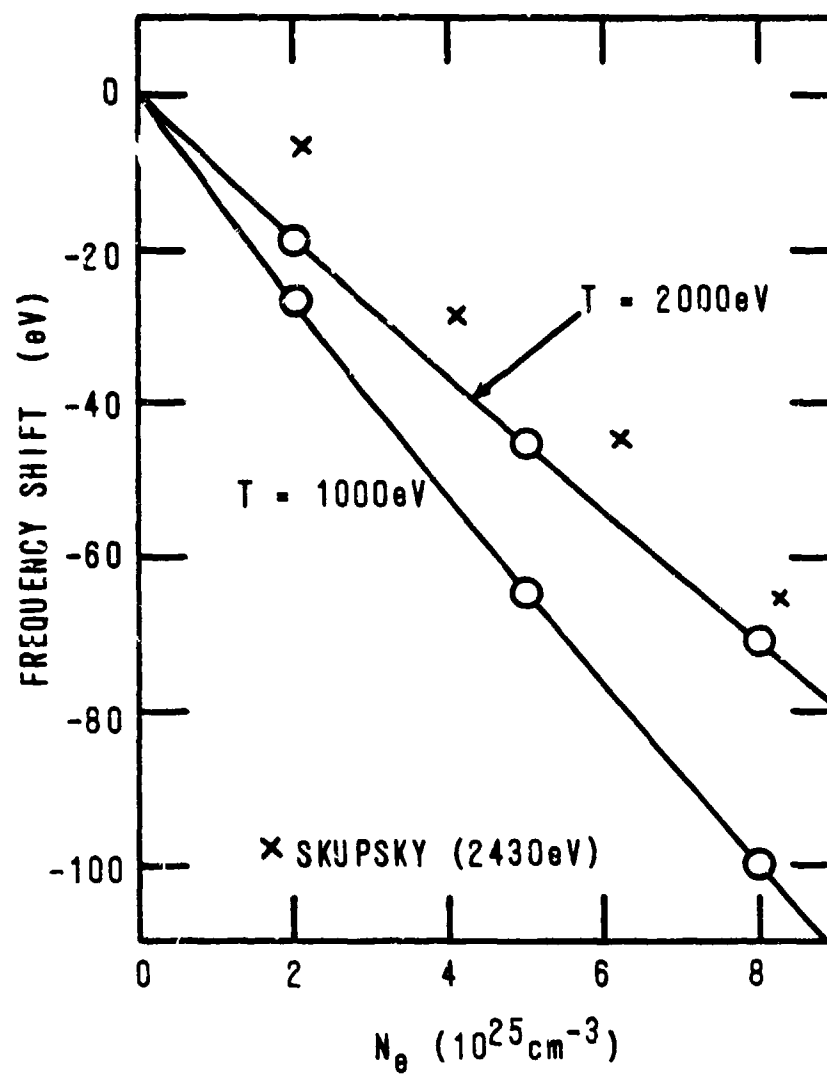


Figure 5. Density dependence of the Ar XVIII Lyman - α line shift.

Table 2

$$A(2p \rightarrow 1s)/A_{\text{Coul}}(2p \rightarrow 1s)$$

	T(eV)	$N_e \text{ (cm}^{-3}\text{)}$		
		10^{24}	3×10^{24}	6×10^{24}
Ne X	200	0.967	0.904	0.840
	500	0.981	0.942	0.887
		$N_e \text{ (cm}^{-3}\text{)}$		
		2×10^{25}	5×10^{25}	8×10^{25}
Ar XVIII	1000	0.950	0.879	0.816
	2000	0.967	0.919	0.873

We have calculated collision strengths for the $1s - 2s$, $1s - 2p$, and $2s - 2p$ transitions of Ne^{+9} and Ar^{+17} using the formalism of the distorted-wave method without exchange. Excitation energies and atomic wave functions were taken from our self-consistent calculations and the equation for the radial functions of the colliding electron were solved using the self-consistent potential (2). However, the modification of the potential of mutual interaction r_{12}^{-1} cannot be properly described within the formalism of the distorted-wave approximation, unless the wave functions of plasma electrons take into account correlation effects between the bound and the free electrons. The variational expression for the element of the reactance matrix then contains an additional term that partially cancels the term of direct Coulomb interaction r_{12}^{-1} as a result of decreased local density of plasma electrons in the vicinity of the bound electron. One can approximate this effect by using the free electron wave functions without correlation and replacing r_{12}^{-1} in the matrix element by $r_{12}^{-1} f(r_{12})$, where $f(r_{12})$ is a properly defined screening function.

$r_{12}^{-1} f(r_{12})$ can be expanded in the form

$$r_{12}^{-1} f(r_{12}) = r_{>}^{-1} \sum_{\lambda=0}^{\infty} P_{\lambda}(\cos \omega) \sum_{\mu=0}^{\infty} A_{\lambda\mu}(r_{>}) (r_{<}/r_{>})^{\lambda+2\mu}, \quad (15)$$

where ω is the angle between \vec{r}_1 and \vec{r}_2 and the coefficients $A_{\lambda\mu}$ depend on the form of $f(r_{12})$.

To demonstrate the effect of screening of the mutual interaction, we have adopted a Debye-Huckel form of the screening function. The expansion (15) have the form

$$\begin{aligned} r_{12}^{-1} \exp(-r_{12}/D) = & \left[r_{>}^{-1} + \frac{1}{6} (r_{>}/D)^2 (r_{<}^2/r_{>}^3) + \dots \right] \exp(-r_{>}/D) P_0(\cos \omega) \\ & + \left[(1 + r_{>}/D) (r_{<}/r_{>}^2) + \frac{1}{10} (1 + r_{>}/D) (r_{>}/D)^2 (r_{<}^3/r_{>}^4) + \dots \right] \\ & \times \exp(-r_{>}/D) P_1(\cos \omega) + \dots \end{aligned} \quad (16)$$

The results for selected values of T and N_e are shown on Figs. 6-11. Also

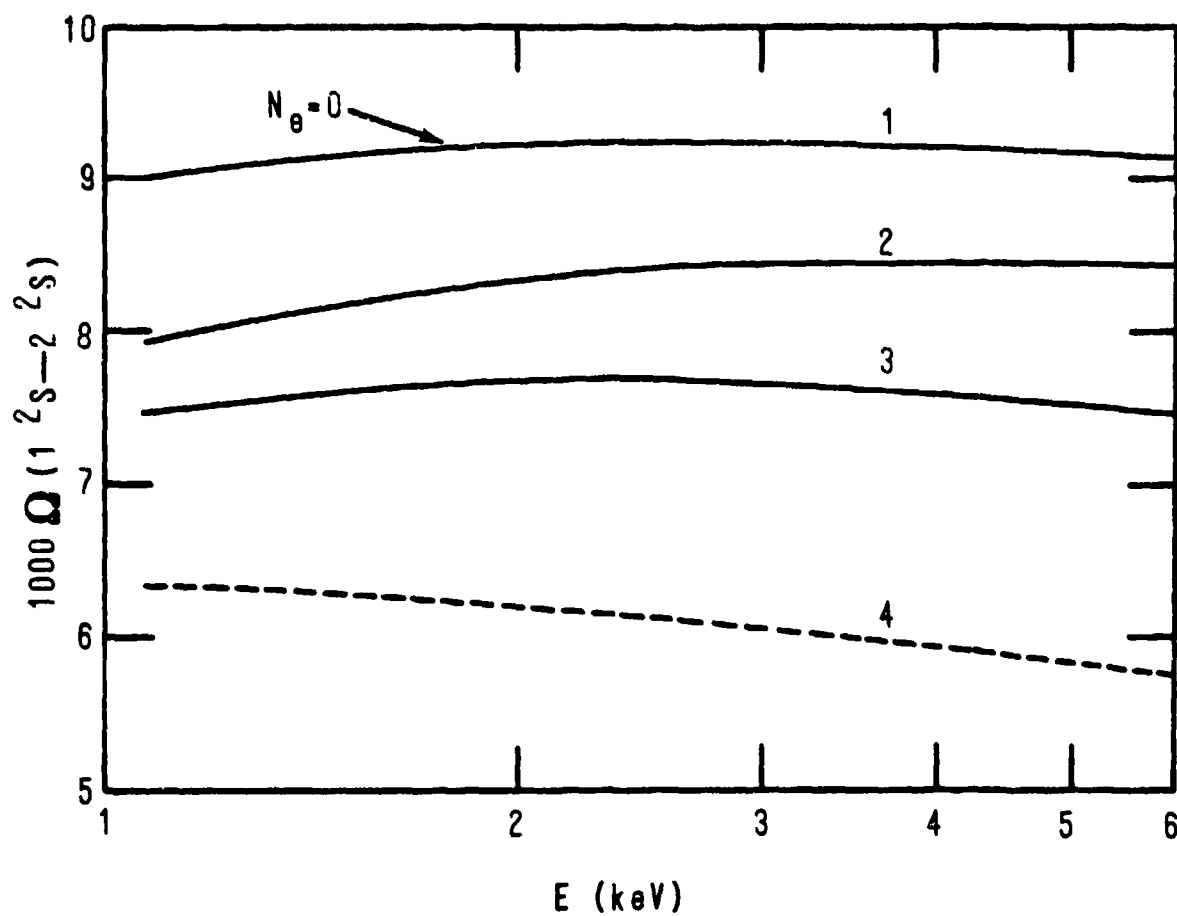


Figure 6. Collision strength Ω ($1s^2S, 2s^2S$) for Ne^{+9} . $T = 200$ eV.
 1 - $N_e = 0$; 2,3,4 - $N_e = 3 \times 10^{24} \text{ cm}^{-3}$; 2 - $D = \infty$; 3 - $D = \Lambda$;
 4 - $D = \frac{1}{2} \Lambda$ (Λ - Debye length).

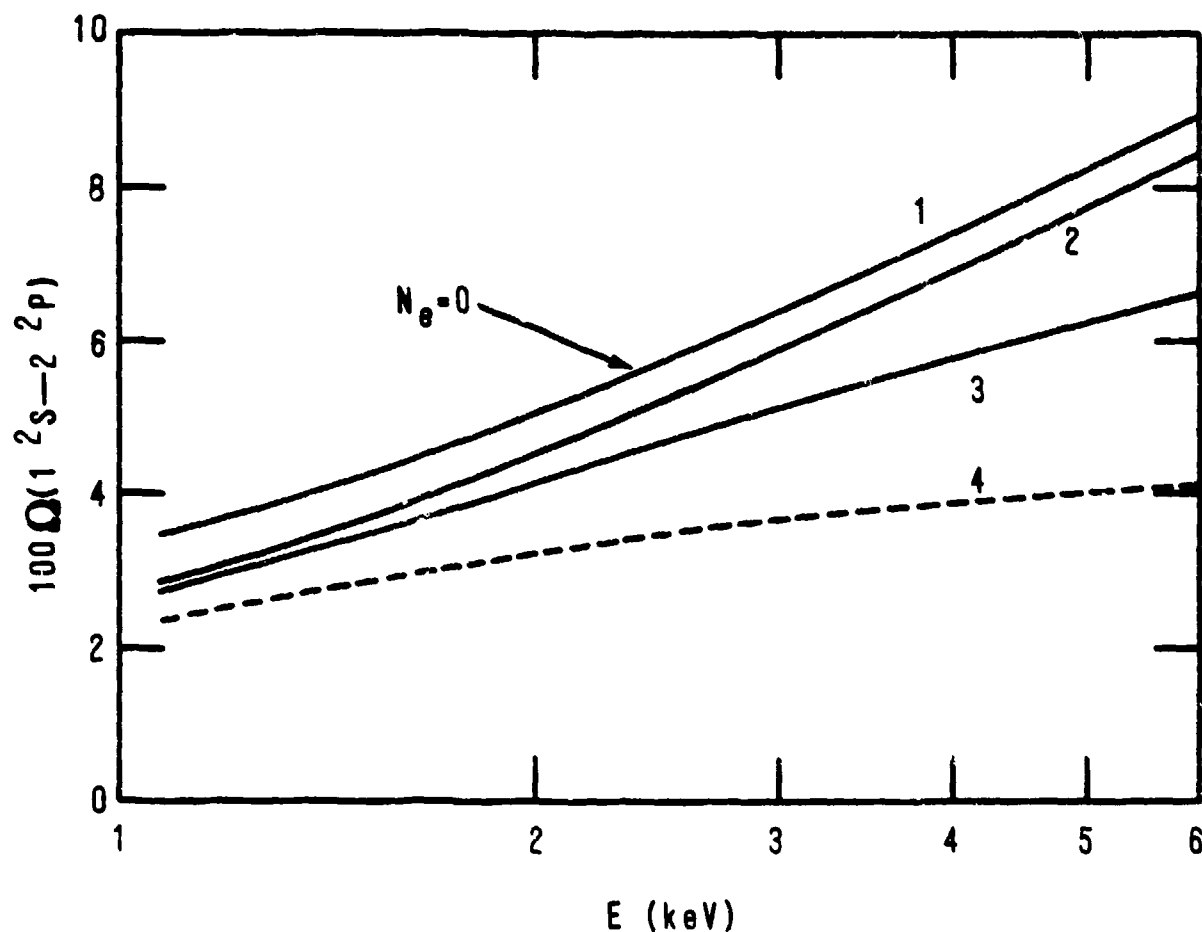


Figure 7. Collision strength $\Omega(1s^2S, 2p^2P)$ for Ne^{+9} . $T = 200 \text{ eV}$.

1 - $N_e = 0$; 2,3,4 - $N_e = 3 \times 10^{24} \text{ cm}^{-3}$; 2 - $D = \infty$; 3 - $D = \Lambda$;
 4 - $D = \frac{1}{2} \Lambda$ ($\Lambda = \text{Debye length}$).

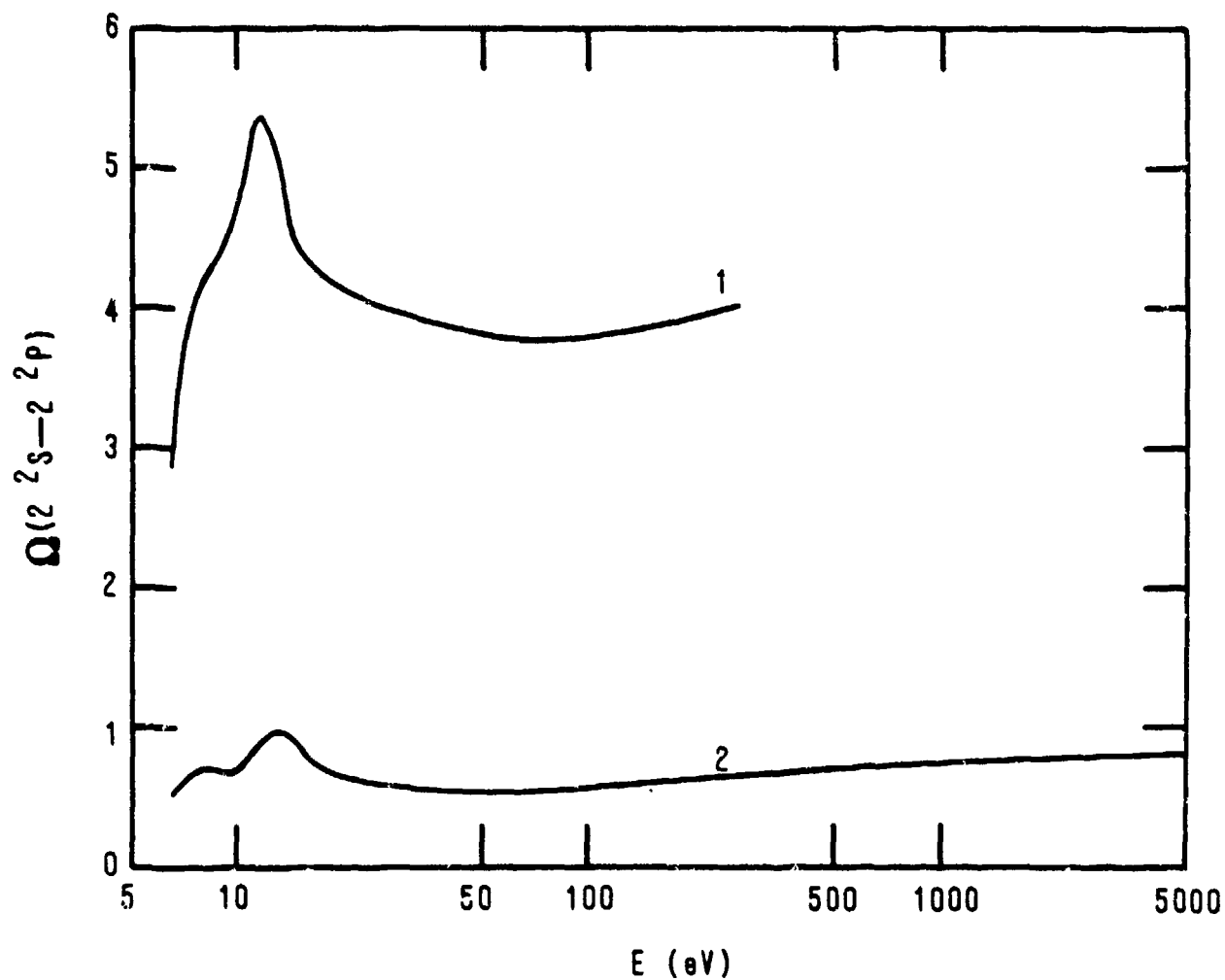


Figure 8. Collision strength $\Omega(2s^2S, 2p^2P)$ for Ne^{+9} . $T = 200$ eV;
 $N_e = 3 \times 10^{24} \text{ cm}^{-3}$. 1 - $D = \infty$; 2 - $D = \text{Debye length}$.

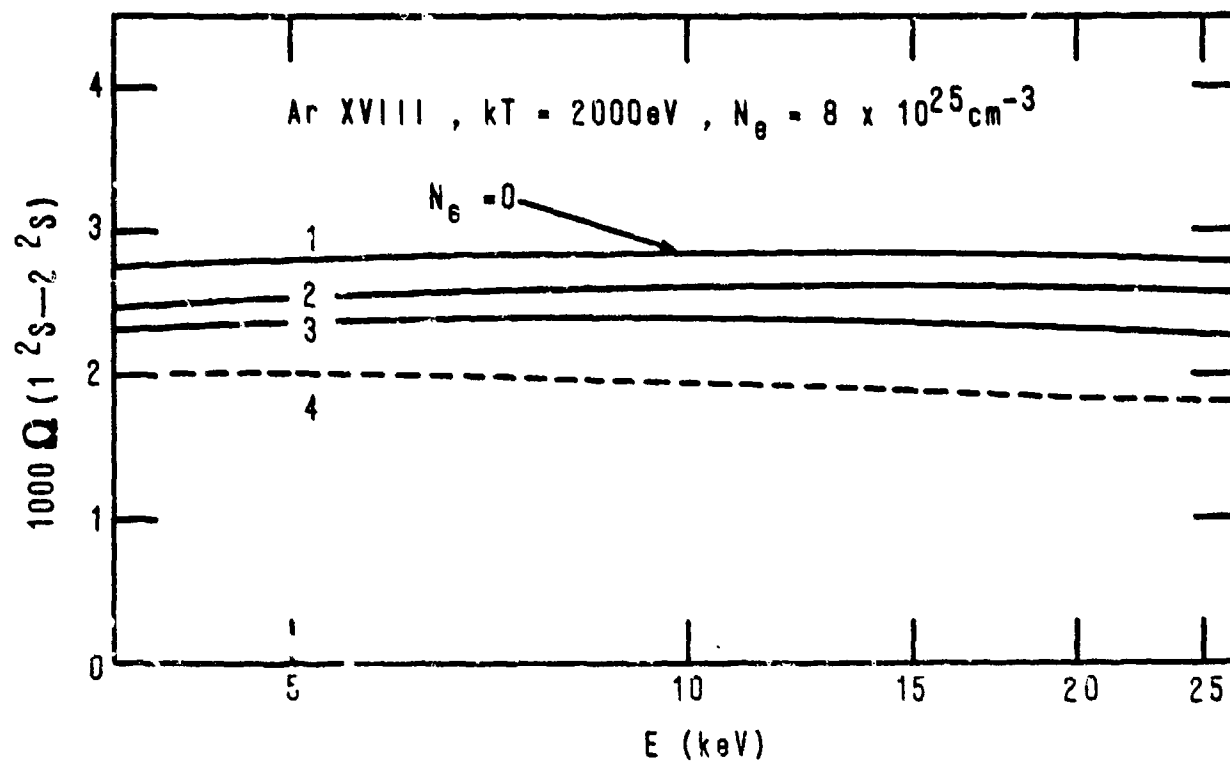


Figure 9. Collision strength Ω ($1s^2S, 2s^2S$) for Ar^{+17} . $T = 2000 \text{ eV}$.

1 - $N_e = 0$; 2, 3, 4 - $N_e = 8 \times 10^{25} \text{ cm}^{-3}$; 2 - $D = \infty$;
 3 - $D = \Lambda$, 4 - $D = \frac{1}{2}\Lambda$ (Λ - Debye length).

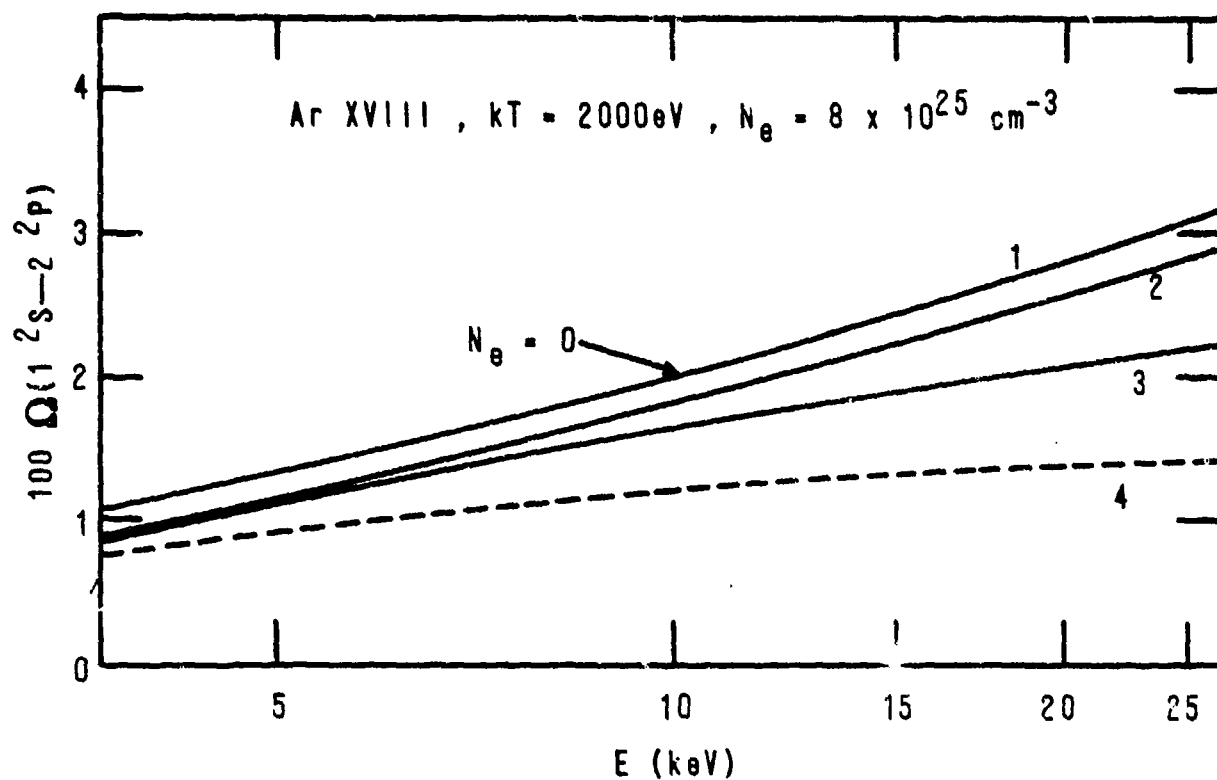


Figure 10. Collision strength $\Omega(1s^2S, 2p^2P)$ for Ar^{+17} . $T = 2000 \text{ eV}$.

1 - $N_e = 0$; 2,3,4 - $N_e = 8 \times 10^{25} \text{ cm}^{-3}$; 2 - $D = \infty$;
 3 - $D = \Lambda$; 4 - $D = \frac{1}{2} \Lambda$ ($\Lambda = \text{Debye length}$).

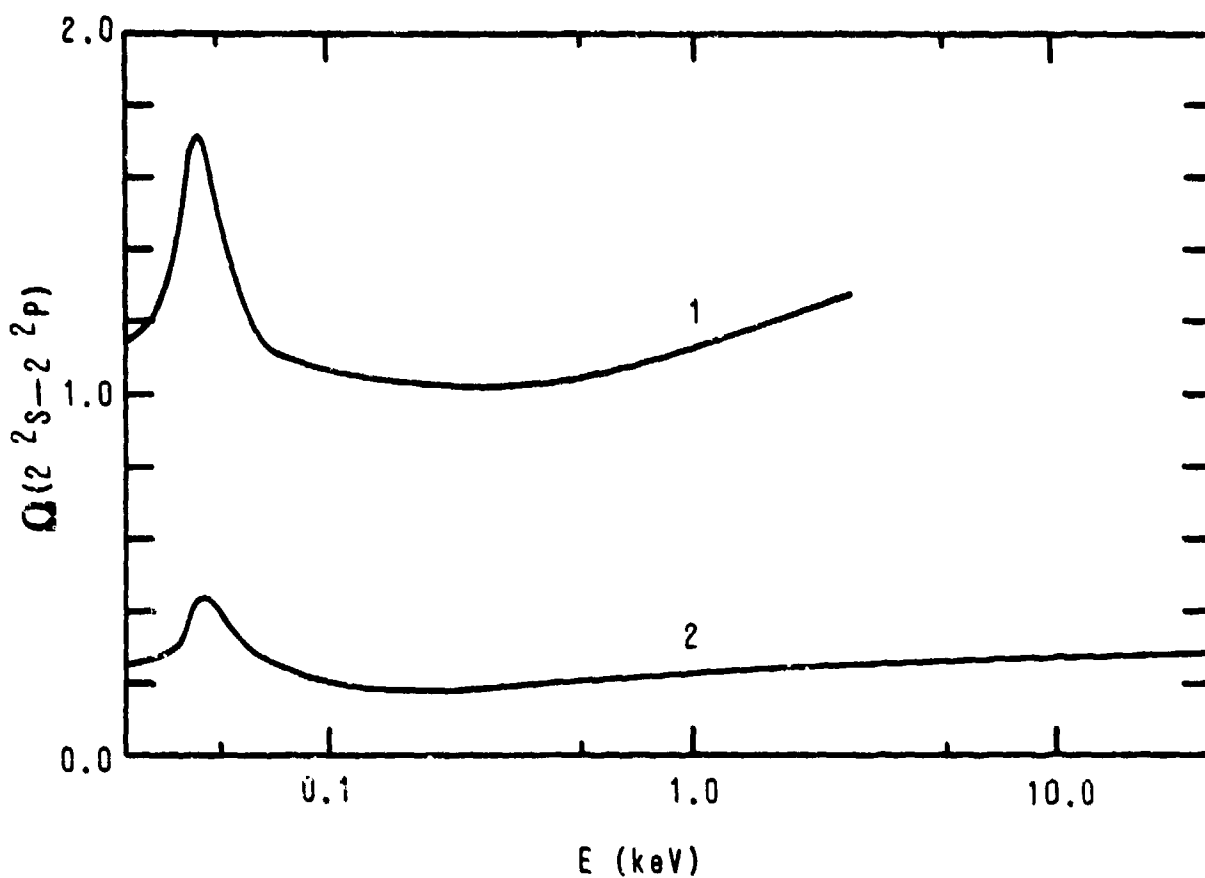


Figure 11. Collision strength $\Omega(2s^2S, 2p^2P)$ for Ar^{+17} . $T = 2000$ eV;
 $N_e = 8 \times 10^{25} \text{ cm}^{-3}$. 1 - $D = \infty$; 2 - $D = \text{Debye length}$.

shown are the collision strengths without any plasma effects ($N_e = 0$) for the transitions $1s - 2s$, $1s - 2p$. The change of atomic wave functions by plasma polarization has a very small effect on the cross sections for conditions considered in this investigation. The change of excitation energies produces a negligible effect on the $1s - 2s$ and $1s - 2p$ transitions but it removes the degeneracy of the $2s$ and $2p$ levels and reduces the $2s - 2p$ cross sections to finite values. For the $1s - 2s$ and $1s - 2p$ transitions, calculations were made for 3 values of the screening parameter D in (16). $D = \infty$ corresponds to the situation where the modification of mutual interaction is ignored and the lowering of the collision strength is caused only by the defocusing of colliding electrons (curve 2 on Figs. 6, 7, 9, 10). Curves 3 and 4 were obtained with $D = \Lambda$ and $D = 1/2 \Lambda$, where Λ is the Debye length for the corresponding temperature and density.

The effect of screening on partial collision strengths increases with increasing angular momentum (Fig. 12) and therefore the dipole transition $1s - 2p$ is more affected than the monopole transition $1s - 2s$. The term corresponding to $\mu = 1$ in the expression (15) and (16) has only a very small effect on the collision strengths.

Collision strengths for the $2s - 2p$ transition were calculated for $D = \infty$ and $D = \Lambda$. The sensitivity of Ω to the value of D is much greater than for the $1s - 2s$ and $1s - 2p$ transitions, because the excitation energy is much smaller, many more partial waves contribute to Ω at a given energy and higher angular momenta are more affected by screening. Collision strengths exhibit a resonance-like behavior in the low-energy region above the excitation threshold. The enhancement of Ω is caused almost exclusively by the contribution from the $\ell = 2, 3$ incident partial waves in Ne^{+9} and by $\ell = 3$ in Ar^{+17} .

IV. RESULTS FOR HYDROGEN AND IONIZED HELIUM

At the present time, there are no experimental data that could be compared with the theoretical results for Ne^{+9} and Ar^{+17} . Therefore we have extended the calculations to neutral hydrogen and singly ionized helium which have been studied experimentally. Unfortunately, the measurement of plasma polarization shifts is a difficult problem and results of various experiments do not always agree with each other. Moreover, the measured shifts represent

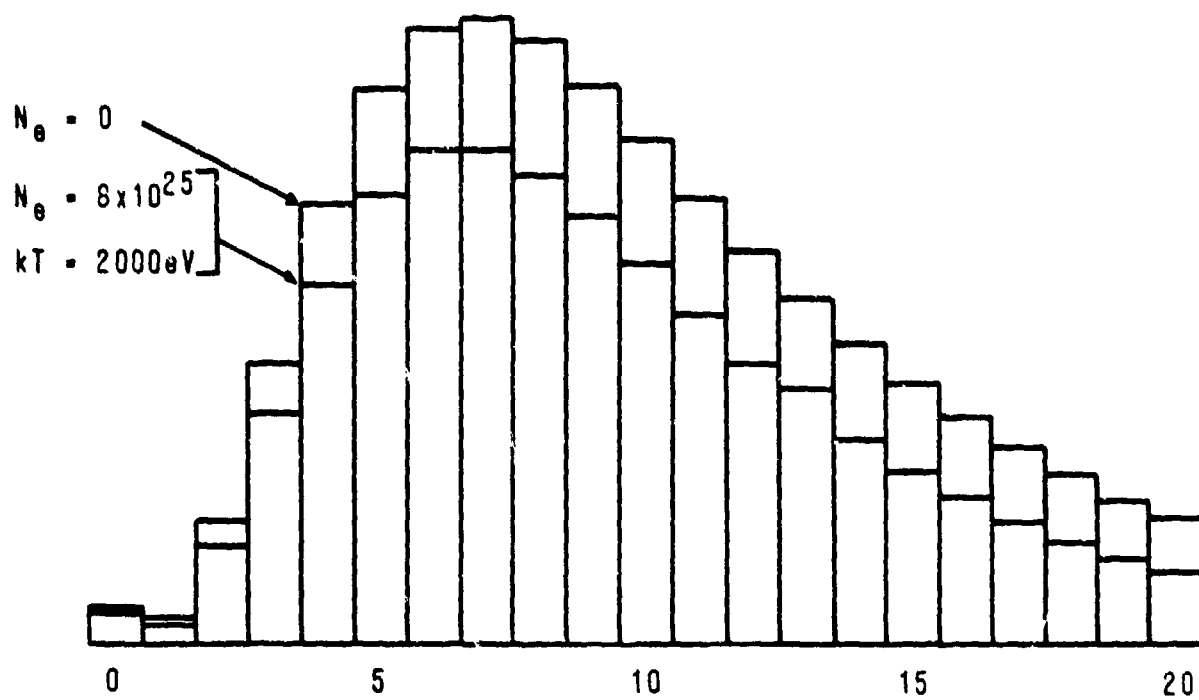


Figure 12. Comparison of partial contributions to the collision strength Ω ($1s^2S, 2p^2P$) for Ar^{+17} for $N_e = 0$ and $N_e = 8 \times 10^{25} \text{ cm}^{-3}$, $T = 2000 \text{ eV}$, $D = \Lambda$.

a combined effect of plasma polarization (i.e. space charges around the atom), ion quadrupole shifts, quadratic Stark effect and shift arising from electron collisions. These additional effects have been ignored in our present investigation and therefore our results for H and He^+ have only a qualitative character.

The plasma conditions in which neutral hydrogen and ionized helium radiate correspond to such low electron densities ($\lesssim 10^{17} \text{ cm}^{-3}$) that several substantial simplifications in our theoretical treatment are possible. In the limit of low charge density (due to plasma electrons and positive ions in the vicinity of the radiating atom) we may omit the effect of these space charges on the motion of free electrons and we solve eq. (8) with $V_{\text{ex}} = V_{\text{corr}} = 0$ and with V from (2) with $\rho_e = \rho_p = 0$. ρ_b is again given by (1), but due to the low temperature, the population of excited levels is so small that it may be omitted altogether.

We will consider pure hydrogen and pure helium plasma and for the sake of simplicity we will assume that the fraction of doubly ionized helium ions is very small. Then all positive ions are singly ionized and we may replace ρ_p by ρ_i in eq. (2) - (4). For the positive charge distribution we again adopt eq. (4) and in order to demonstrate the effect of different ion distributions on level shifts we use three different forms of V : (a) $V = 0$ which corresponds to a uniform ion distribution, (b) V calculated from (2) with $\rho_e = \rho_p = 0$ and with ρ_b from (1) assuming that only the $1s$ level is occupied. (c) V from (2) with $\rho_e = \rho_p = 0$ and ρ_b from (1) assuming that only the level $n\ell$, for which the shift is being calculated, is occupied. This last choice may find a justification if we compare de Broglie wavelength λ_B for thermal electrons and ions: while λ_B for electrons is comparable or larger than the dimensions of the atom and therefore plasma electrons do not adjust to individual atomic states $n\ell$, λ_B for ions is much smaller and the ion distribution may depend on $n\ell$. In using eq. (4) for the ion distribution, one should employ, of course, the true interatomic potential V . This potential may be substantially different, especially for hydrogen, from the potential we are using the present work. This is another reason why our results should be compared with experiment only with caution.

The level shifts in the low-density limit are calculated from the perturbation expression

$$\Delta E_{nl} = - \int_0^{\infty} P_{nl}^2 V' dr, \quad (17)$$

where $V' = V - Zr^{-1}$ and V is calculated from (2) with $\rho_b = 0$, $\rho_p = \rho_i$ and with ρ_i and ρ_e obtained by the procedure just described. In the low-density limit we do not perform self-consistent calculations and therefore we do not know the correct behavior of V at large distances. Consequently we cannot carry out the integration in (17) up to the indicated upper limit and cannot calculate absolute level shifts as in the high density case. However, we can obtain relative shifts $\Delta E_{nl} - \Delta E_{n'l'}$, if we integrate, in (17), up to the distance beyond which all radial functions P_{nl} involved in the calculation vanish.

From (17) it follows that level shifts are proportional to electron density N_e . As a consequence, we do not have to perform a thermal average of electron density distribution before calculating the potential from (2) and shifts from (17), but instead we can first calculate shifts for the charge distribution corresponding to a given velocity of electrons and perform the thermal average of these shifts. They are a smooth function of electron velocity and the average can be obtained with great accuracy.

We have obtained relative level shifts for all nl levels of H and He^+ with $n = 1$ to 4. Weighted averages over the l - values for each principal quantum number n , normalized to the density $N_e = 10^{17} \text{ cm}^{-3}$ are displayed on Figs. 13 and 14. Relative level shifts for H are more sensitive to the choice of the ion distribution than for He^+ .

For He^+ , our results predict a very small red shift of Lyman series lines. The experimental evidence, however, points to a much larger blue shift². Theoretical blue shifts were derived by Greig et al.⁹, Burgess and Peacock¹⁰ and Volonté¹¹, but the apparent agreement of all these theoretical results with experiment is basically due to the omission of space charges outside the orbit of the bound electron, and this assumption does not appear to be properly justified.

For the 3 - 2 transition of He^+ at 1640 Å our theory predicts a negligible red shift in agreement with experiment, but the theoretical shift for the 4 - 2 transition at 1215 Å is again too small, except possibly for the temperature around 4 eV.

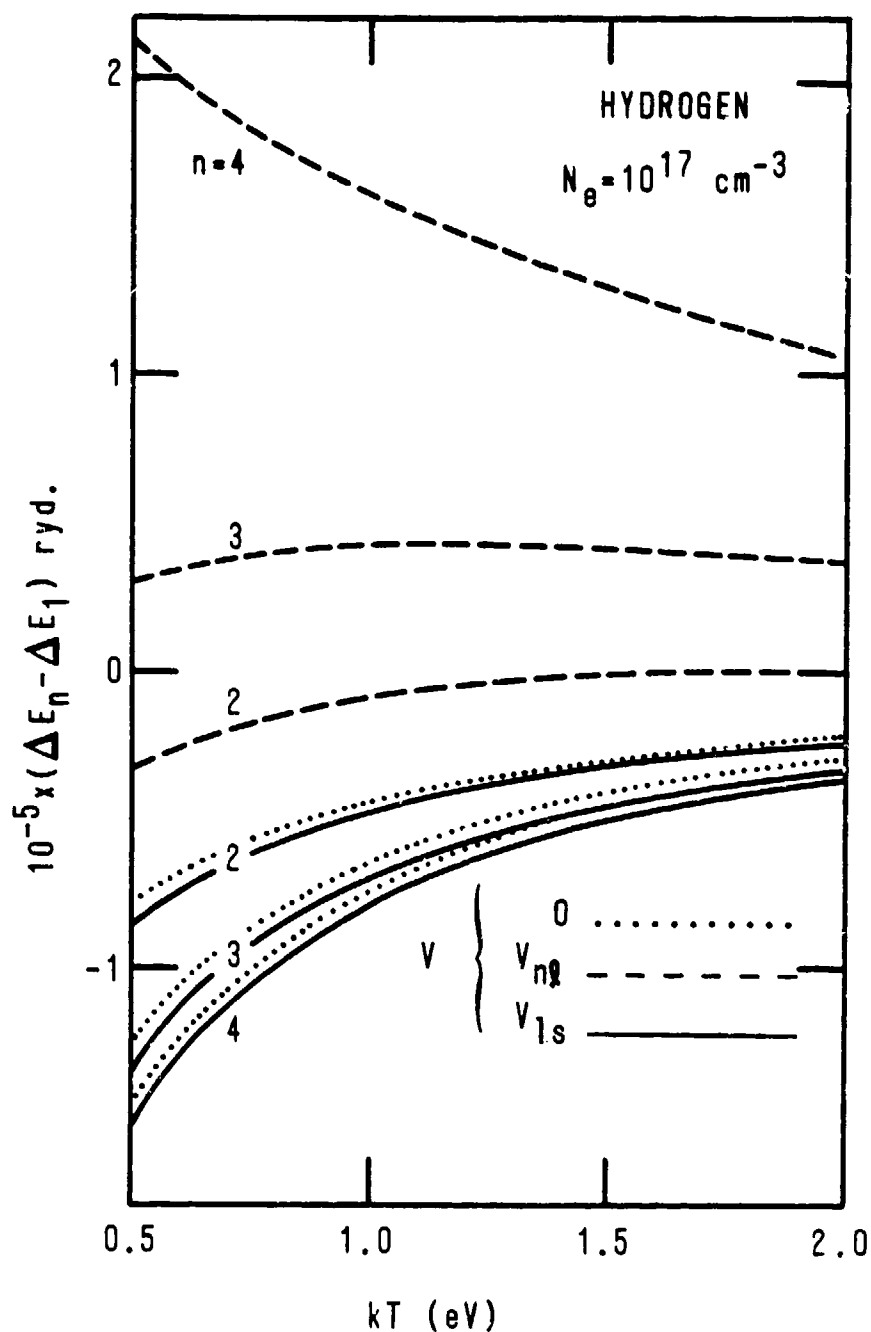


Figure 13. Temperature dependence of relative level shifts for hydrogen. Dotted lines: uniform ion distribution (ion density obtained from eq. (4) with $V=0$). Broken lines: ion density given by eq. (4) with V derived from screening by the $n\ell$ electron. Solid line: ion density given by eq. (4) with V derived from screening by the $1s$ electron.

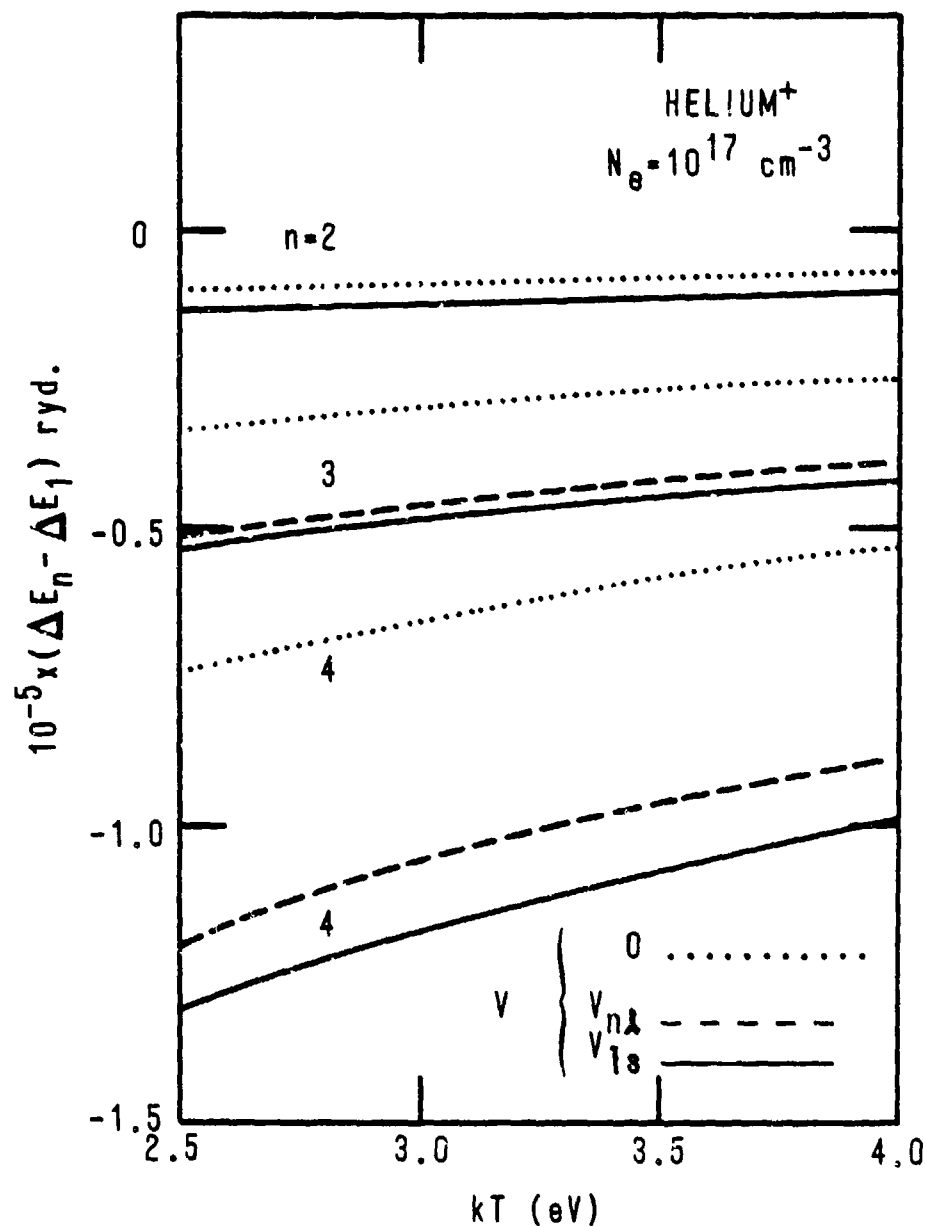


Figure 14. Temperature dependence of relative level shifts for helium⁺
Dotted lines: uniform ion distribution (ion density obtained from eq. (4) with V=0). Broken lines: ion density given by eq. (4) with V derived from screening by the nl electron. Solid line: ion density given by eq. (4) with V derived from screening by the 1s electron.

Pittman et al.¹² measured a red shift of 0.17 \AA for the transition $4 - 3$ at 4686 \AA for $T = 4 \text{ eV}$. From Fig. 14 we find shifts of 0.07 , 0.12 and 0.14 \AA for three different ion distributions. This may be considered a satisfactory agreement with respect to the uncertainty of the ion distribution.

The same authors also measured red shifts of the Balmer series lines of neutral hydrogen. Our theoretical results predict either much smaller values or even blue shifts, but an agreement can hardly be expected due to the very approximate form of the ion distribution.

For reasons mentioned earlier, the comparison with experiment is generally very inconclusive. The theoretical treatment should be improved first of all by using correct ion distribution and by properly taking into account other effects leading to the shifts of atomic levels.

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REFERENCES

1. H. R. Griem, Proc. 7th Int. Conf. on Phenomena in Ionized Gases, Belgrade, Yugoslavia (1965).
2. M. Neiger and H. R. Griem, Phys. Rev. A 14, 291 (1976).
3. J. R. Van Zandt, J. C. Adcock, and H. R. Griem, Phys. Rev. A 14, 2126 (1976).
4. O. Theimer and P. Kepple, Phys. Rev. A 1, 957 (1970).
5. B. F. Rozsnyai, J. Quant. Spectrosc. Radiat. Transfer 15, 695 (1975); Phys. Rev. A 5, 1137 (1972).
6. S. Skupsky, Phys. Rev. A 21, 1316 (1980).
7. M.W.C. Dharma-wardana, private communication (1980).
8. M.W.C. Dharma-wardana and R. Taylor, J. Phys. C: Solid St. Phys. 13, XXX (1980).
9. J. R. Greig, H. R. Griem, L. A. Jones, and T. Oda, Phys. Rev. Lett. 24, 3 (1970).
10. D. D. Burgess and N. J. Peacock, J. Phys. B4, L94 (1971).
11. S. Volonté, J. Phys. B8, 1170 (1975).
12. T. L. Pittman, P. Voigt, and D. E. Kelleher, Phys. Rev. Lett. 45, 723 (1980).

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